Spectral Barriers in Certification Problems

Dmitriy (Tim) Kunisky — Dissertation Defense

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I. Introduction

Our Question:

Are there efficient algorithms to certify bounds on random optimization problems?

Main example:

$$\mathsf{M}(\boldsymbol{W}) := \max_{\boldsymbol{x} \in \{\pm 1\}^n} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}$$

(including Sherrington-Kirkpatrick and other Ising-type Hamiltonians, max-cut in graphs, synchronization over $\mathbb{Z}/2\mathbb{Z}$, etc.)

General *constrained PCA* problem:

$$\mathsf{M}_{\mathcal{X}}(\boldsymbol{W}) := \max_{\boldsymbol{X} \in \mathcal{X}} \mathsf{Tr}(\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X})$$

(including Potts and vector-spin Hamiltonians; graph coloring; some CSPs; tensor, sparse, positive, conic, and other PCAs; etc.)

Search and Certification

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Search: Compute $\boldsymbol{x}_{\mathsf{alg}} = \boldsymbol{x}_{\mathsf{alg}}(\boldsymbol{W})$ with large value of objective $\boldsymbol{x}_{\mathsf{alg}}^{\top}\boldsymbol{W}\boldsymbol{x}_{\mathsf{alg}}$.

- Local ("greedy") search (or Markov chains, simulated annealing)
- Projected power method (or AMP variants)
- Relax and round

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Certification: Compute small $c(\boldsymbol{W}) \in \mathbb{R}$ that gives a bound $\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x} \leq c(\boldsymbol{W})$ *for all* feasible $\boldsymbol{x}$.

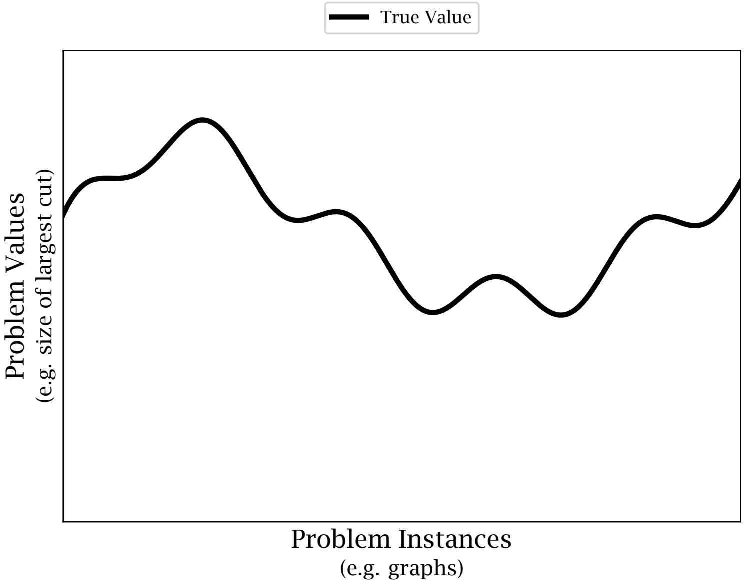
- LP relaxations (metric, Sherali-Adams, Lovász-Schrijver)
- SDP relaxations (Goemans-Williamson, **sum-of-squares/Lasserre**)

Search and Certification: Objective Bounds

$$\boldsymbol{x}_{\mathsf{alg}}^{\top} \boldsymbol{W} \boldsymbol{x}_{\mathsf{alg}} \quad \leq \quad \mathsf{M}(\boldsymbol{W}) \quad \leq \quad c(\boldsymbol{W})$$

search	certification
$\updownarrow$	$\updownarrow$
lower bounds	**upper** bounds

Average-Case Analysis



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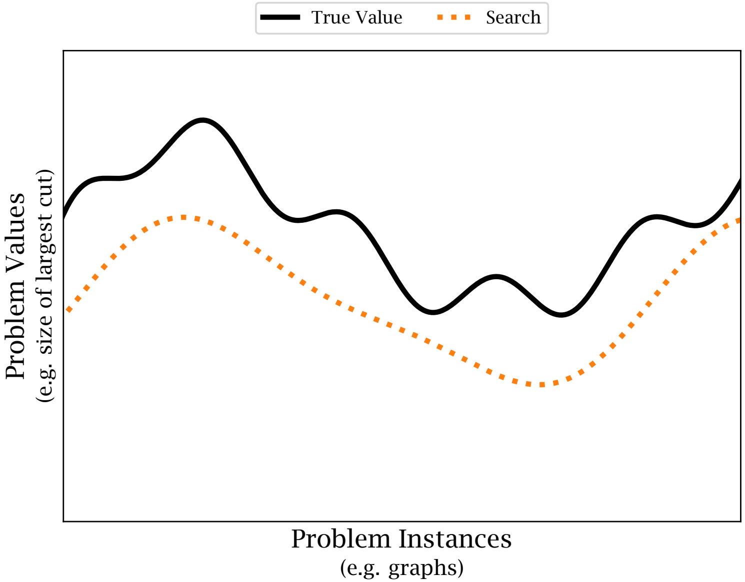

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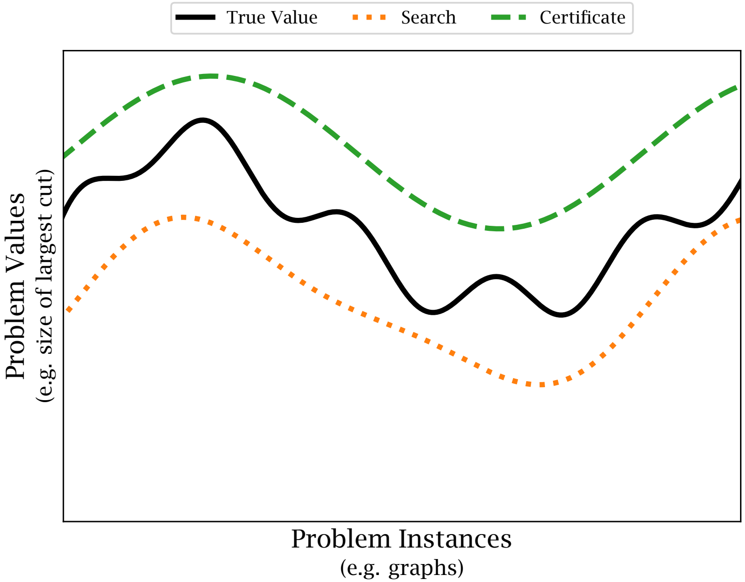

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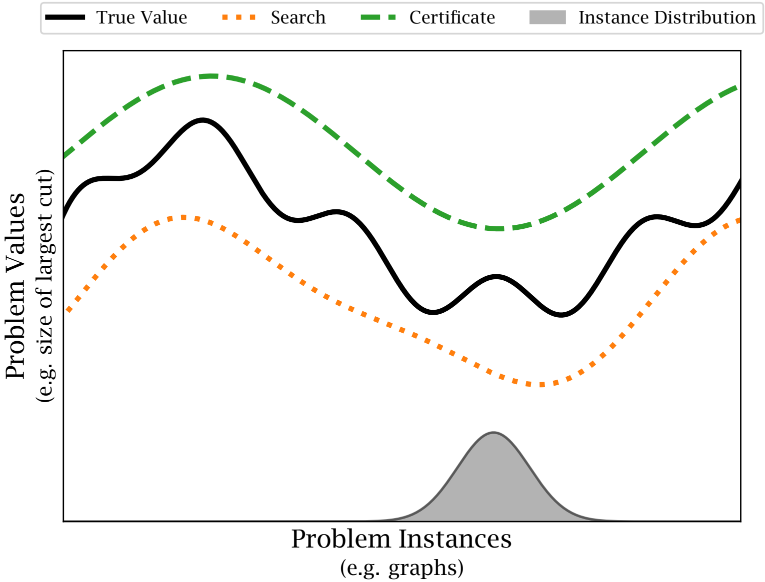

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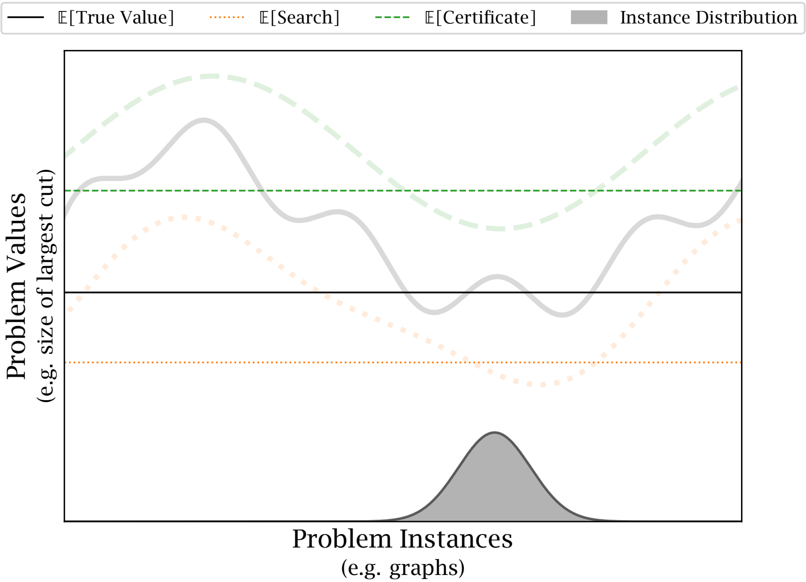

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Take $\mathsf{M}(\boldsymbol{W}) = \mathsf{max}_{\boldsymbol{x} \in \{\pm 1\}^n} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}$, for random $\boldsymbol{W} \sim \mathsf{GOE}(n)$.

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Statistical physics tells us the true value:

$$\lim_{n \to \infty} \mathbb{E}\mathsf{M}(W)/n = 2\mathsf{P}_* \approx 1.526,$$ (“Parisi number”)

ground state of the SK model. [SK ’75; Parisi ’79; Guerra, Talagrand ’00s]

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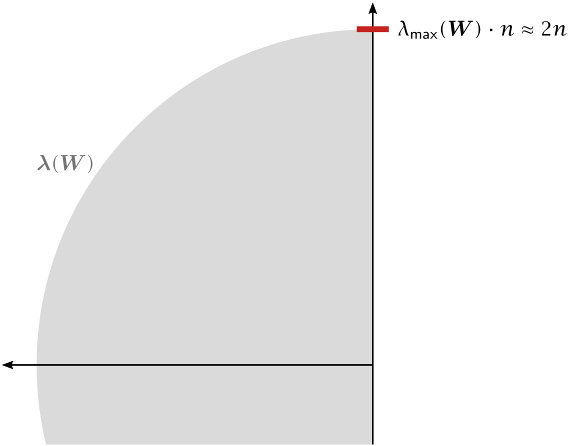
Other reasons to care:

- Natural sparse random graph limit
  [Boettcher, Zdeborová '10; Montanari, Sen '16; Dembo, Montanari, Sen '17]
- Proof complexity of ground state bounds (will see later)
- Mean width of cut polytope $\mathrm{conv}(\{\boldsymbol{x}\boldsymbol{x}^\top : \boldsymbol{x} \in \{\pm 1\}^n\})$

Searching for Hypercube in the GOE Spectrum



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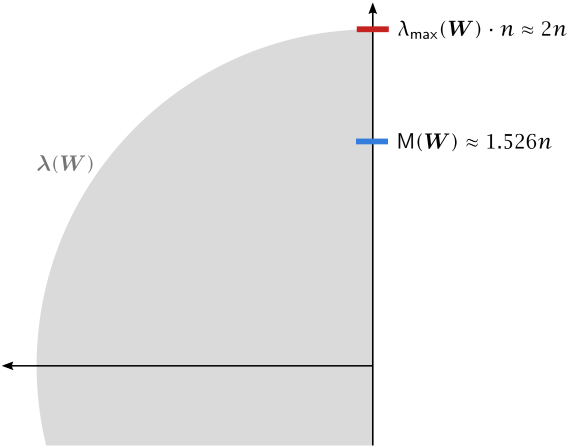

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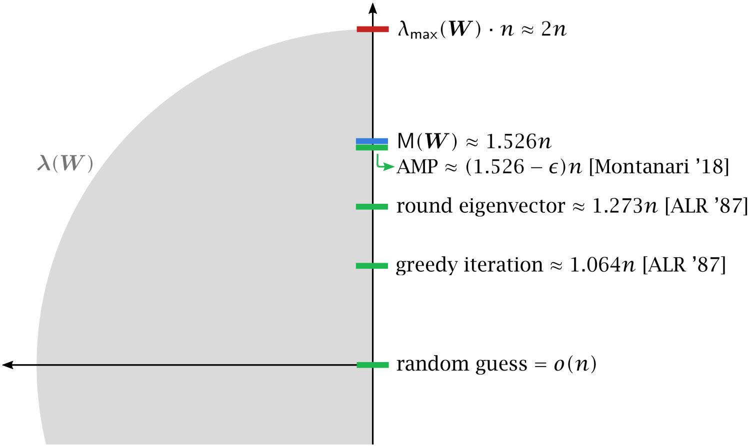

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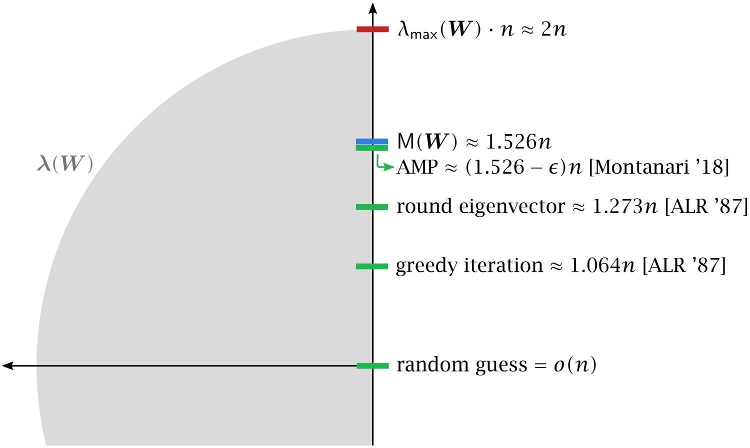

Optimal search! And certification?

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The simplest way to bound $\mathsf{M}(\boldsymbol{W})$: ignore all special structure in $\boldsymbol{x}$, to get

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\mathsf{M}(\boldsymbol{W}) &= \max_{\boldsymbol{x} \in \{\pm 1\}^n} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x} \\
&\leq \max_{\|\boldsymbol{x}\| = \sqrt{n}} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x} \\
&= \lambda_{\mathsf{max}}(\boldsymbol{W}) \cdot n \\
&\approx 2n, \qquad \text{(for } \boldsymbol{W} \sim \mathsf{GOE}(n)\text{)}
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Can we do better?

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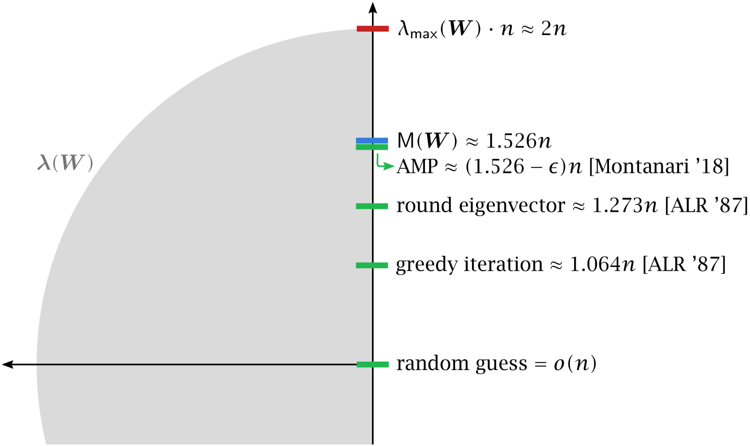

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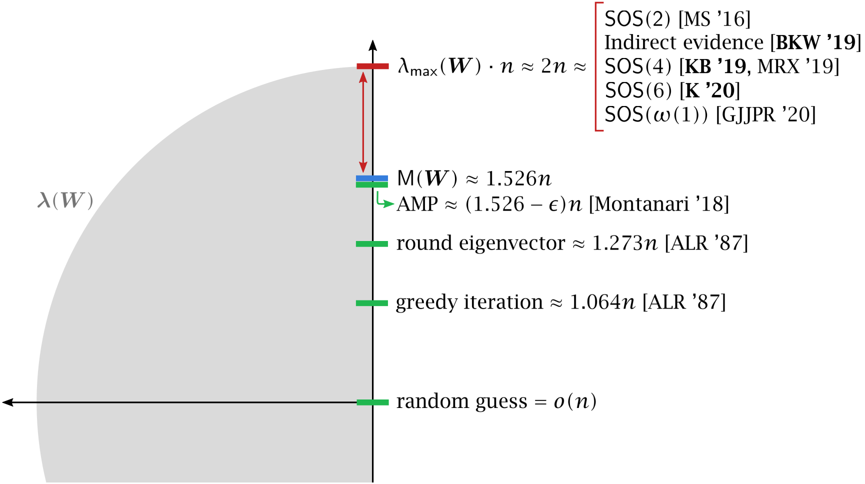

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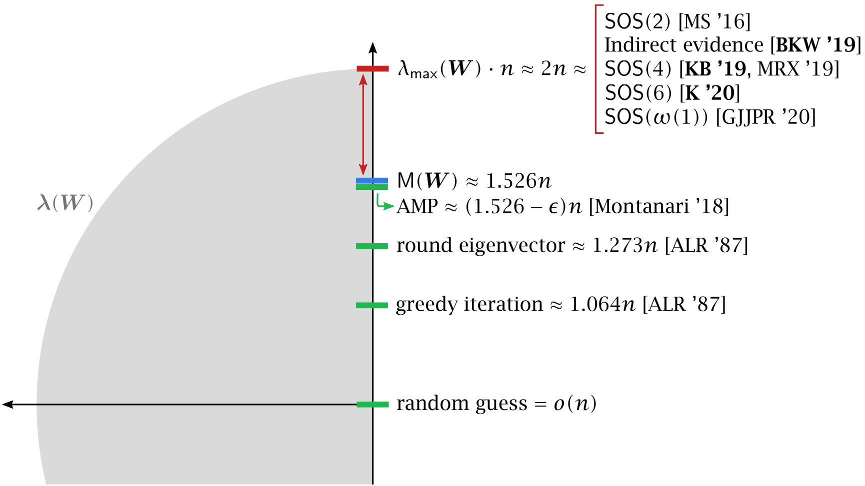

Optimal search, but **spectral barrier** to certification.

II. Computationally-Quiet Planting

Implicit Hypothesis Testing [WBP '16, BKW '19]

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Lemma (Reduction): Can certify $c(\boldsymbol{W}) \le (2 - \epsilon)n$ w.h.p. $\Rightarrow$ in same amount of time can test w.h.p. between:

1. $\boldsymbol{Y} \sim \mathbb{Q}_n$ (null model),
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models of eigenspaces of $\boldsymbol{W}$.

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Corollary (Hardness of Certification): If low-degree polynomial algorithms are optimal tests, then no algorithm running in time $\exp(O(n^{1-\delta}))$ certifies $c(\boldsymbol{W}) \leq (2-\epsilon)n$.

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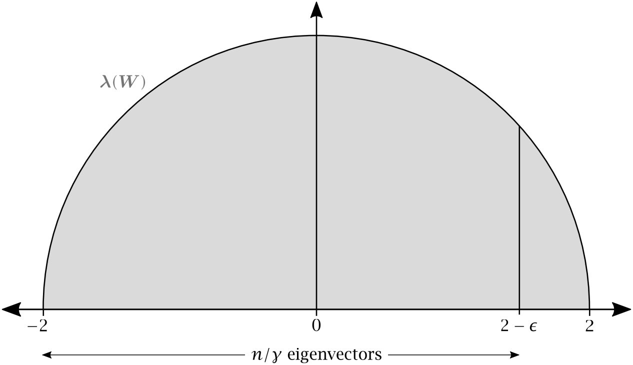
GOE bottom eigenspaces vs. avoiding $\boldsymbol{x} \sim \mathsf{Unif}(\{\pm 1\}^n)$:

1. $\boldsymbol{y}_1, \dots, \boldsymbol{y}_{\frac{n}{\gamma}} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}) \rightsquigarrow$ GOE,
2. $\boldsymbol{y}_1, \dots, \boldsymbol{y}_{\frac{n}{\gamma}} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I} - \frac{\beta}{n}\boldsymbol{x}\boldsymbol{x}^\top) \rightsquigarrow$ spectrally-planted GOE.



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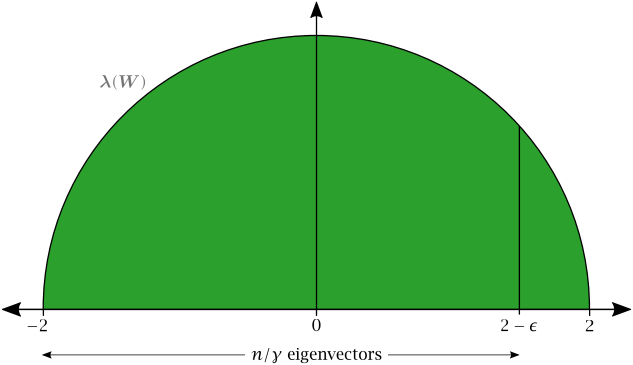

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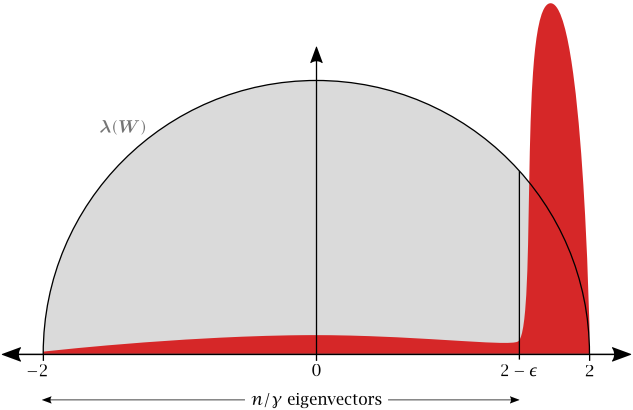

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This is a **Wishart (negatively) spiked matrix model.**

[Johnstone '01, BBAP '05, BS '06, ...] but negative case first appreciated by [PWBM '18]

Gaussianity $\rightsquigarrow$ can do explicit calculations to assess difficulty of testing.

Similar versions for general setting: different or higher-rank constraints $\mathcal{X}$ with random $\boldsymbol{X}$ near $\mathcal{X}$.

[BBKMW '20, BKW '20, Chapter 2 of thesis]

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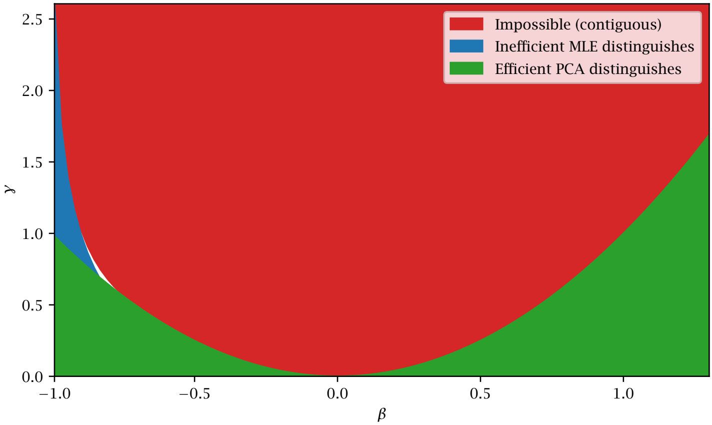

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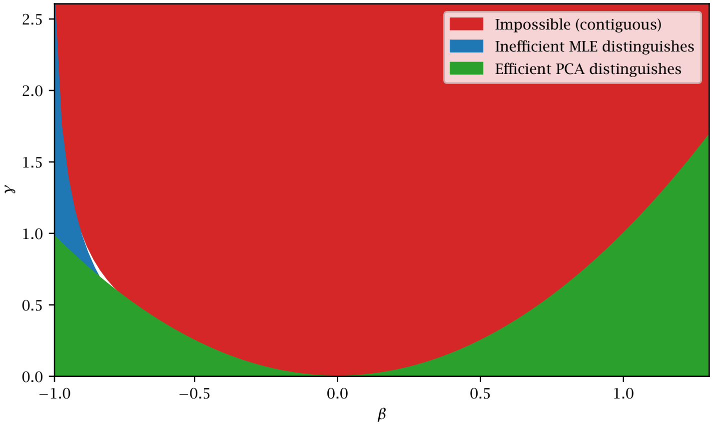

Better evidence of hardness than just PCA failure?

Low-Degree Tests [HKPRSS '17, HS '17, Hopkins '18]

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Take {low-degree polynomials} ≈ {efficient algorithms}, and compute:

$$\begin{aligned} \text{maximize} \quad & \mathbb{E}_{\mathbb{P}_n}\, p(\boldsymbol{Y}) \\ \text{subject to} \quad & \mathbb{E}_{\mathbb{Q}_n} p(\boldsymbol{Y})^2 \le 1, \\ & p(\boldsymbol{Y}) \in \mathbb{R}[\boldsymbol{Y}]_{\le D}. \end{aligned}$$

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Optimizer: the (normalized) **low-degree likelihood ratio**

$$p^\star(\boldsymbol{Y}) = \mathcal{P}^{\le D} \frac{d\mathbb{P}_n}{d\mathbb{Q}_n}(\boldsymbol{Y}) \;\Big/\; \underbrace{\left\| \mathcal{P}^{\le D} \frac{d\mathbb{P}_n}{d\mathbb{Q}_n} \right\|}_{\text{objective value}}.$$

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Conjecture: Cannot test in time $e^{\widetilde{O}(D(n))}$ if objective $= O(1)$.

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New evidence for hard or subexponential regimes in:

- Dense matrix PCA (Wigner/**Wishart**, rank k, many priors) [BKW ’19]
- One special non-Gaussian dense matrix PCA [K ’20]
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From Wishart models + reduction, conclude conditional hardness of better-than-spectral certification in:

- SK Hamiltonian ("Gaussian max-cut") [BKW '19]
- Potts glass Hamiltonian ("Gaussian coloring") [BBKMW '20]
- Positive PCA ("Gaussian max-clique") [BKW '20]

Unified Proofs from Overlap Formulae

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Algebraic simplification of orthogonal polynomials method: when in planted $\mathbb{P}_n$ we observe noisy signal $\widetilde{\boldsymbol{X}}$ (e.g. $= \boldsymbol{x}\boldsymbol{x}^\top$),

$$\left\| \mathcal{P}^{\leq D} \frac{d\mathbb{P}_n}{d\mathbb{Q}_n} \right\|^2 = \sum_{|\boldsymbol{\alpha}| \leq D} \left\langle q_{\boldsymbol{\alpha}}, \frac{d\mathbb{P}_n}{d\mathbb{Q}_n} \right\rangle^2 \leq \mathop{\mathbb{E}}_{\widetilde{\boldsymbol{X}}^1, \widetilde{\boldsymbol{X}}^2} \sum_{d=0}^{D} c_d \, r(\widetilde{\boldsymbol{X}}^1, \widetilde{\boldsymbol{X}}^2)^d$$

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Reduce to contest of low-dimensional **replica overlap** $r(\tilde{\boldsymbol{X}}^1, \tilde{\boldsymbol{X}}^2)$ tails vs. **link function** $f(t) = \sum_{d=0}^{\infty} c_d t^d$ growth.

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Model	**Overlap**	**Link Function**
Gaussian Wigner	$\langle\widetilde{\boldsymbol{X}}^1,\widetilde{\boldsymbol{X}}^2\rangle$	$\exp(t)$
Morris Exp. Families	$\langle\boldsymbol{z}(\widetilde{\boldsymbol{X}}^1),\boldsymbol{z}(\widetilde{\boldsymbol{X}}^2)\rangle$	$(1-vt)^{-1/v}$
Gaussian Wishart	$\widetilde{\boldsymbol{X}}^1\widetilde{\boldsymbol{X}}^2$	$\det(\boldsymbol{I}-\boldsymbol{T})^{-n/2\gamma}$

III. Sum-of-Squares Lower Bounds

State of Affairs So Far

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Reduction + low-degree analysis $\rightsquigarrow$ evidence of no efficient better-than-spectral certification algorithm.

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1. $\boldsymbol{W} \sim$ something other than $\mathsf{GOE}(n)$; in particular, analysis **without exact law of eigenvectors**.

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1. $\boldsymbol{W} \sim$ something other than $\mathsf{GOE}(n)$; in particular, analysis **without exact law of eigenvectors**.

2. **Concrete lower bounds** rather than “evidence” conditional on conjecture re: low-degree polynomials.

Sum-of-Squares Relaxations [Parrilo '00, Lasserre '01]

A way to design increasingly powerful **semidefinite programming** relaxations of $\mathsf{M}(\boldsymbol{W}) = \max_{\boldsymbol{x} \in \{\pm 1\}^n} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}$.

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$$
\begin{aligned}
\max \quad & \widetilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] \\
\text{s.t.} \quad & \widetilde{\mathbb{E}} : \mathbb{R}[x_1, \dots, x_n]_{\leq D} \to \mathbb{R} \\
& \widetilde{\mathbb{E}} \text{ linear} \\
& \widetilde{\mathbb{E}}[1] = 1 \\
& \widetilde{\mathbb{E}}[(x_i^2 - 1) p(x)] = 0 \\
& \widetilde{\mathbb{E}}[s(x)^2] \geq 0
\end{aligned}
$$

pseudoexpectation,
imposter,
charlatan,
...

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pseudoexpectation,
imposter,
charlatan,
...

sum-of-squares prover,
detective,
tester,
...

Sum-of-Squares Relaxations [Parrilo '00, Lasserre '01]

A way to design increasingly powerful **semidefinite programming** relaxations of $\mathsf{M}(\boldsymbol{W}) = \max_{\boldsymbol{x} \in \{\pm 1\}^n} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}$.

$$
\begin{array}{ll}
\max & \widetilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] \\
\text{s.t.} & \widetilde{\mathbb{E}} : \mathbb{R}[x_1, \dots, x_n]_{\leq D} \to \mathbb{R} \\
& \widetilde{\mathbb{E}} \text{ linear} \\
& \widetilde{\mathbb{E}}[1] = 1 \\
& \widetilde{\mathbb{E}}[(x_i^2 - 1) p(x)] = 0 \\
& \widetilde{\mathbb{E}}[s(x)^2] \geq 0
\end{array}
\quad = \quad
\begin{array}{ll}
\min & c \\
\text{s.t.} & c - \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x} \\
& \quad = \sum_i p_i(x)(x_i^2 - 1) \\
& \quad + \sum_j s_j(x)^2 \\
& \deg p_i \leq D - 2 \\
& \deg s_j \leq D/2
\end{array}
$$

pseudoexpectation, imposter, charlatan, ...

sum-of-squares prover, detective, tester, ...

Pay runtime of $n^{\Theta(D)}$ for flexibility of degree D proofs.

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Choosing $\widetilde{\mathbb{E}}$ = choosing each $\widetilde{\mathbb{E}}[x_{i_1} \cdots x_{i_D}]$, starting with $\widetilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top] \propto$ projector to top eigenspace V of $\boldsymbol{W}$. ($D = 2$ [MS '16])

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Use planted distribution ("$\boldsymbol{x} \in V \cap \{\pm 1\}^n$") to determine these, entry by entry. Only difficulty: **proving positivity**.

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Question: Whose **Gram matrices** are these large structured psd matrices? How to make more explicit these **geometric** objects underlying SOS lower bounds?

Spectral Extensions [BK '18, KB '19, K '20]

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Probabilistic viewpoint: use *surrogate random tensors*,

$$\widetilde{\mathbb{E}}[\boldsymbol{x^i x^j}] := \mathbb{E}[G_{\boldsymbol{i}}^{(d)} G_{\boldsymbol{j}}^{(d)}] \quad \leftrightarrow \quad \text{“}\boldsymbol{G}^{(d)} = \boldsymbol{x}^{\otimes d}\text{”}$$

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Make $\boldsymbol{G}^{(d)}$ as random as possible under constraints—give it a canonical Gaussian distribution conditional on:

$$G_{\emptyset}^{(0)} = 1 \quad \leftrightarrow \quad x^{\otimes 0} = (1)$$

$$\boldsymbol{G}^{(d)} \text{ symmetric} \quad \leftrightarrow \quad x_{i_1} \cdots x_{i_d} = x_{\pi(i_1)} \cdots x_{\pi(i_d)}$$

$$G_{j,j,i_1,\dots,i_{d-2}}^{(d)} = G_{i_1,\dots,i_{d-2}}^{(d-2)} \quad \leftrightarrow \quad x_j^2 \boldsymbol{x}^{\boldsymbol{i}} = \boldsymbol{x}^{\boldsymbol{i}}$$

$$(G_{j,i_1,\dots,i_{d-1}}^{(d)})_{j=1}^{n} \in V \quad \leftrightarrow \quad x_{i_1} \cdots x_{i_{d-1}} \boldsymbol{x} \in V$$

for V top eigenspace of $\boldsymbol{W}$.

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With homogeneous polynomials $\rightsquigarrow$ ideal generated by $\langle \boldsymbol{P}_V \boldsymbol{e}_i, \boldsymbol{z} \rangle^2$ and *multiharmonic* polynomials $\langle \boldsymbol{P}_V \boldsymbol{e}_i, \boldsymbol{\partial} \rangle^2 p = 0$.

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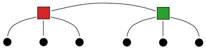
Multiharmonic projections $\rightsquigarrow$ Green's function representation gives diagrammatic expressions. [Maxwell 1873!]

$\widetilde{\mathbb{E}}[x_i x_j x_k x_\ell x_m x_p]$ = sum of expressions of the form

$P_{ij} P_{k\ell} P_{mp}$

$P_{ij} \sum_{a=1}^{n} P_{ak} P_{a\ell} P_{am} P_{ap}$



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Möbius function coefficients $\rightsquigarrow$ identities "explaining" compatibility of positivity and entry symmetries.

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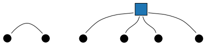
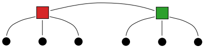
$P_{ij}P_{k\ell}P_{mp}$

1



$P_{ij} \sum_{a=1}^{n} P_{ak}P_{a\ell}P_{am}P_{ap}$

−2



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With spectral extensions:

- Deterministic analysis of degree 4 feasible set [BK '18]
- Degree 4 lower bound for SK Hamiltonian [KB '19]
- Towards higher-degree lower bounds: [K '20]
  - Degree 6 lower bound for SK Hamiltonian
  - Degree $\omega(1)$ for incoherent high-rank projector
- Spectrum of parity $\widetilde{\mathbb{E}}$ [Grigoriev '01, Laurent '03, BKM '21]

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Meanwhile, with pseudocalibration:

- Degree 4 lower bound for SK Hamiltonian [MRX '19]
- Degree $\omega(1)$ lower bound for SK Hamiltonian [GJJPR '20]

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- Spectra and Gramian structure of pseudoexpectations
- Pseudocalibration reconciliation
- Proof systems for spin glasses—replicated SOS? [RS ’00]

Thank you!